MYCOBACTERIUM TUBERCULOSIS CYP130: CRYSTAL STRUCTURE, BIOPHYSICAL CHARACTERIZATION, AND INTERACTIONS WITH ANTIFUNGAL AZOLE DRUGS *

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SUPPLEMENTAL FIGURES

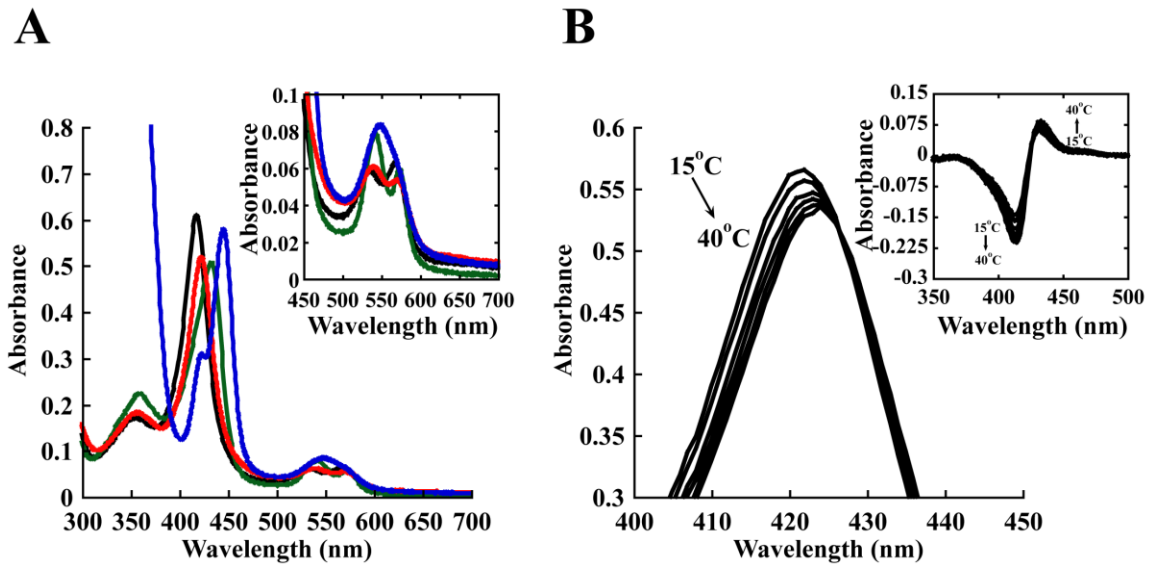

Fig S1**. UV-visible absorption spectra of CYP130.** *A*, absorption spectra for ferric CYP130 (5 µM) in the oxidized (black line), econazole-bound (red line), NO-bound (green line) and ferrous CO-bound (blue line) CYP130 forms. The insert in panel *A* is an enlargement of the visible region. *B*, temperature dependence of the degree of econazole interaction with heme. CYP130 (5 µM) complexed with econazole (25 µM) was incubated at 15, 20, 25, 30, 35 and 40 °C. The inset of panel *B* shows the difference spectra of econazole-bound-*minus*-ligand-free CYP130 recorded at each temperature.

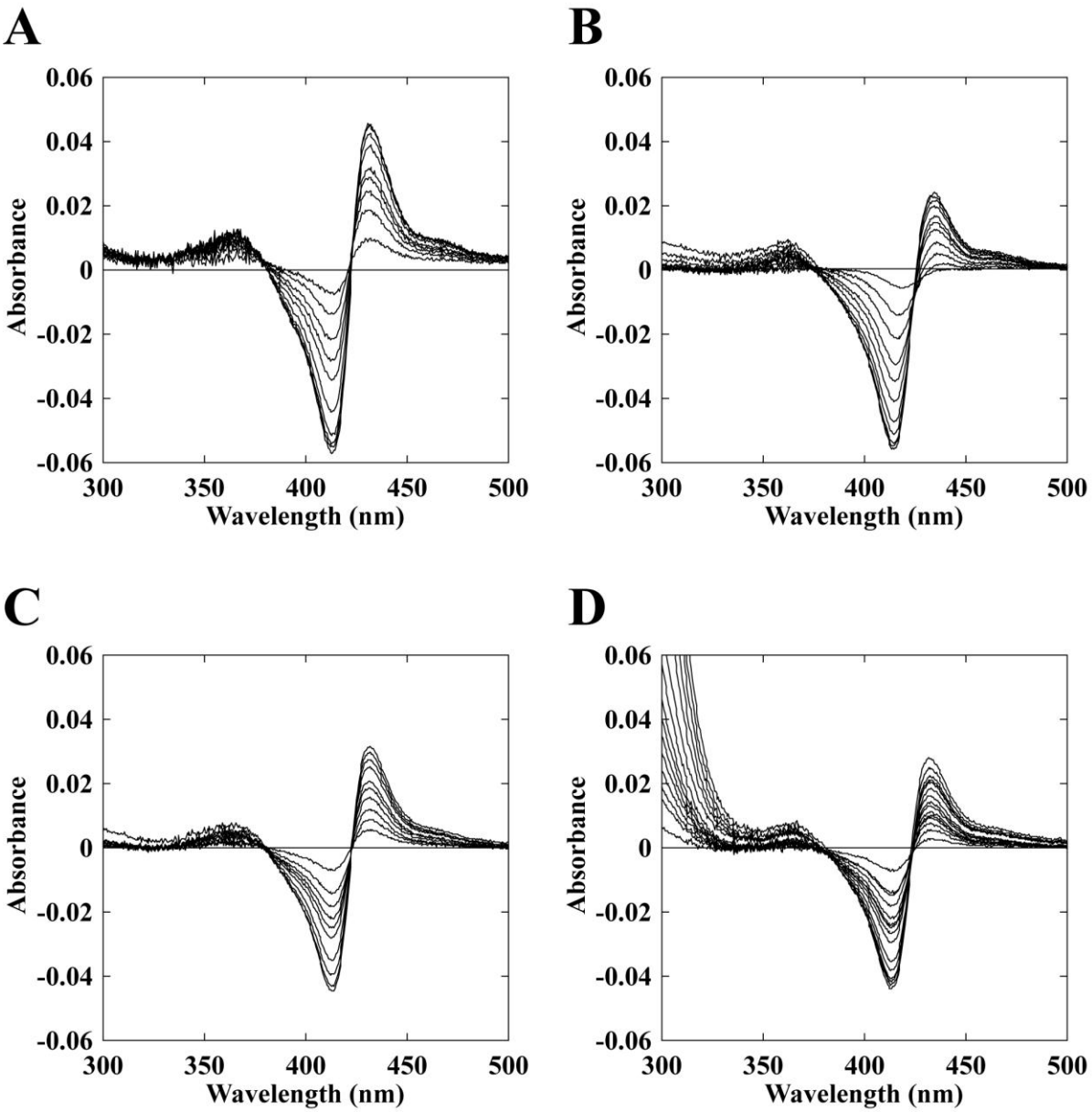

Fig S2. **Representative difference spectra of ligand-bound-*minus*-ligand-free CYP130**. The protein (2.5 µM) was titrated at 23 °C with econazole (A), clotrimazole (B), miconazole (C) and ketoconazole (D).

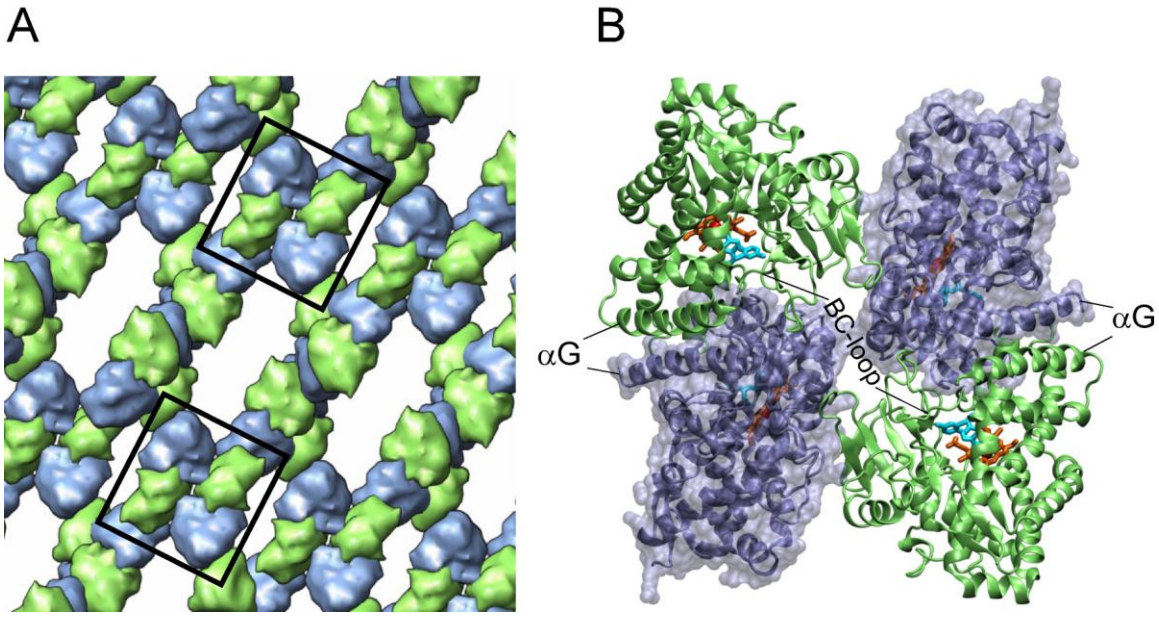

Fig. S3. **Packing of the CYP130/econazole complex in the crystal.** *A*, a fragment of the crystal lattice which is largely stabilized via formation of the protein tetramer (enclosed in black squares) is shown. Copies of each chain in the dimer are colored in blue and green. Figure was generated using CHIMERA program. *B*, zoom-in on CYP130 tetrameric structure derived from the crystal. One set of monomers is highlighted by the transparent surfaces.